PR-18. INVESTIGATION OF THE STRUCTURE AND PROPERTIES OF VITAMINS AND HORMONES

A. S. Shipilova, A. V. Knyazev, E. V. Gusarova, A. A. Amosov, S. S. Knyazeva, A. E. Kortikova

Lobachevsky University, Gagarin Av., 23/2, Nizhny Novgorod, 603950, Russia

E-mail: 28_stasy@bk.ru

The aim of this work is the creation of a technological basis for the development and production of biologically active substances (BAS), namely, vitamins and hormones, valuable for medicine, agriculture, chemical, food and microbiological industry. This goal can be achieved by studying of the physico-chemical properties and structural-functional relationships of biological objects by methods such as, vacuum adiabatic calorimetry, combustion calorimetry, x-ray diffraction and other. For the production of synthetic drugs it is necessary to study their properties, which can be used to create and improve existing methods for the production and purification of substances by means of the computer programs. Such programs allow to realize the computer synthesis based on the data on the structure of the compounds, the thermodynamic parameters of substances and the chemical reactions is selected as the main criteria for programming. Study of structural properties and polymorphism has great importance for industry because the polymorphic forms of a drug differ in physico-chemical properties, such as solubility, chemical and physical stability, hygroscopicity, tableting, and biological activity. At the moment we investigated the structural and thermodynamic properties of B vitamins and steroid hormones (Table 1, 2).

Table 1

Thermodynamic characteristics of formation of biologically active substances

Compound	$-\Delta_f H°(298)$ (kJ/mol)	$-\Delta_f S°(298)$ (J/(mol·K))	$-\Delta_f G°(298)$ (kJ/mol)
Riboflavin	1432 ±13	1961 ±3	847 ±14
Nicotinic acid	344,9 ±0,9	503 ±3	195 ±2
Myo-inositol	1329,3 ±2,3	1232,5 ±3,5	962 ±3
Folic acid dihydrate	1821,0 ±5,7	2515,5 ±9,5	1071 ±6
L-carnitine	756,2 ±2,5	1182,5 ±3,5	403,5 ±3
Cyanocobalamin	5017 ±15	7281 ±5	2846 ±15
Methylprednisolone	1045,8 ±7,3	2141 ±11	407 ±8
Methylprednisolone aceponate	1465,3 ±9,8	2592,9 ±13,7	692 ±10
Prednisolone	1020,6 ±7,6	–	–
Hydrocortisone acetate	1307,0 ±11,6	–	–

Table 2

Crystallographic parameters of biologically active substances

Formula	$C_{27}H_{36}O_7$		$C_{23}H_{30}O_6 \cdot C_2H_5OH$	$C_{23}H_{30}O_6 \cdot C_3H_7OH$
Sample	Methylprednisolone aceponate		Ethanol solvates cortisone acetate	Propanol solvates cortisone acetate
Symmetry, Z	Orthorhombic $P2_12_12_1$, 4	Orthorhombic $P2_12_12_1$, 12	Monoclinic $P2_1$, 2	Monoclinic $P2_1$, 2
a, Å	6,57348 (14)	14,8592 (2)	9,6973 (4)	9,8941 (3)
b, Å	14,8295 (3)	19,6844 (5)	7,4950 (3)	7,3833 (2)
c, Å	26,2214 (5)	26,2214 (5)	16,1828 (7)	16,5816 (5)
β, °	–	–	93,559	90,110
V, Å^3	2556,11 (9)	7652,4 (2)	1173,92 (8)	1211,30 (6)